Intermolecular Interaction of Tween 80, Water and Butanol in Micelles Formation via Molecular Dynamics Simulation

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Abstract:
Micelles entrapment approach is one of the methods to synthesize silica nanoparticles as carriers for drug delivery system. This method is useful in enhancing drug solubility, extend the circulation of blood half-life and possesses lower toxicity. The shape and size of the silica nanoparticles could be excellently controlled by manipulating the parameters such as the concentration of surfactants and composition during the synthesis process. In this study, water and butanol have been used as solvent and co-solvent, while Tween 80 has been used as the surfactant. The structural properties of the micellar system from binary (water and Tween 80) and ternary (water, Tween 80 and butanol) were reported in terms of radial distribution function (RDF) and radius of gyration (Rg). The molecular dynamics simulations were performed using Material Studio by applying COMPASS Force Field in the Forcite Module. The simulation box was created by using Amorphous Cell Module. Initially, the simulation for both system was executed under a constant number of moles, volume and energy (NVE) ensemble for 200 ps and followed by a constant number of moles, pressure and temperature (NPT) ensemble for 2000 ps. From RDF analysis, both systems have the same distance of 0.97Å, but different value of g(r) intensity, 12 and 6.35 respectively. Meanwhile, the Rg result shows a higher value in ternary systems compared to the binary system. These findings revealed that the presence of butanol would weaken the intermolecular interaction of hydrogen bond and increase the size of the micelle and consequently will affect the size of nanoparticles.

Keywords: Co-Solvent; Lower Toxicity; Water and Butanol; Molecular Dynamics.

ACKNOWLEDGMENT

The author would like to appreciate the financial support from Universiti Malaysia Pahang through Research Grant Scheme, RDU1703316.